Gaussian wave packet & its spread with time:—

The function

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i[kx-\omega t]}\, dk$$

Here $\phi(k)$ is a Gaussian function given by

$$\phi(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} e^{-a(k-k_0)^2}$$

$$\therefore \psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2} e^{i[kx-\omega t]}\, dk.$$

At $t=0$

$$\psi(x,0) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2} e^{ikx}\, dk \quad \ldots\ (1)$$

Substituting $k' = k-k_0$ we get

$$\psi(x,0) = \int_{-\infty}^{+\infty} e^{-ak'^2} e^{i(k'+k_0)x}\, dk'$$

$$= e^{ik_0x} \int_{-\infty}^{+\infty} e^{-ak'^2} e^{ik'x}\, dk' \quad \ldots\ (2)$$

Now

$$-ak'^2 + ik'x = -\left[ak'^2 - ik'x\right]$$

$$= -a\left[k'^2 - \frac{ik'}{a}x\right]$$

$$= -a\left[(k')^2 - 2.k'\frac{ix}{2a} + \left(\frac{ix}{2a}\right)^2 - \left(\frac{ix}{2a}\right)^2\right]$$

$$= -a\left[\left(k' - \frac{ix}{2a}\right)^2 - \frac{i^2x^2}{4a^2}\right]$$

$$= -a\left(k' - \frac{ix}{2a}\right)^2 - \frac{x^2}{4a}$$

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Putting back in eqn. ②.

$$\psi(x,0) = e^{ik_0x}\int_{-\infty}^{+\infty} e^{-a\left(k'-\frac{ix}{2a}\right)^2} e^{-\frac{x^2}{4a}}\,dk'$$

$$= e^{ik_0x} e^{-x^2/4a}\int_{-\infty}^{+\infty} e^{-a\left(k'-\frac{ix}{2a}\right)^2}\,dk'$$

Let $k' - \frac{ix}{2a} = q$

$\therefore dk' = dq.$

$$\therefore \psi(x,0) = e^{ik_0x} e^{-x^2/4a}\,\frac{\sqrt{\pi}}{\sqrt{a}} \quad \left[\because \int_{-\infty}^{+\infty} e^{-aq^2}dq = \sqrt{\frac{\pi}{a}}\right].$$

$$\boxed{\psi(x,0) = B(x)\,e^{ik_0x}}$$

Here $B(x) \rightarrow$ amplitude of the wavepacket &

$e^{ik_0x} \rightarrow$ phase factor.

$$|\psi(x,0)|^2 = B^2 = \frac{\pi}{a}\, e^{-x^2/2a} \quad \text{---- (2A)}$$

Now $\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2} e^{i[kx-\omega t]}\,dk.$

If $\omega(k) = ck$ i, ω is linear in k.

$$\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2} e^{ik(x-ct)}\,dk \quad \text{--- ③}$$

$$\therefore \boxed{\psi(x,t) = \psi(x-ct,0).}$$

eqn. ③ is similar to equation ① except that x is replaced by $x-ct$.

$$\therefore |\psi(x-ct,0)|^2 = \frac{\pi}{a}\, e^{-\frac{(x-ct)^2}{2a}}.$$

Thus the wavefn. $\psi(x,t) = [\psi(x-ct, 0)]$ have the same shape as that of starting wave fn. $\psi(x,0)$. Thus there is no spreading in time.

But for matter waves, ω is not linearly proportional to k.

$$\omega(k) = \omega(k_0 + k - k_0) \qquad \text{(Taylor expansion)}$$

$$= \omega(k_0) + (k-k_0)\left.\frac{\partial \omega}{\partial k}\right|_{k_0} + \frac{1}{2}(k-k_0)^2\left.\left(\frac{\partial^2 \omega}{\partial k^2}\right)\right|_{k_0} + \cdots$$

$$= \omega(k_0) + (k-k_0)v_g + \frac{1}{2}(k-k_0)^2\beta + \cdots$$

$\omega(k) = \frac{\hbar k^2}{2m}$

$$\psi(x,t) = \int_{-\infty}^{+\infty} e^{-a(k-k_0)^2} e^{i[kx - \omega(k_0)t - (k-k_0)v_g t - \frac{1}{2}\beta (k-k_0)^2 t]} dk$$

Let $k - k_0 = k'$

$\therefore k = k' + k_0$.

$$\therefore \psi(x,t) = \int_{-\infty}^{+\infty} e^{-ak'^2} e^{i[k_0 x + k'x]} e^{-i\omega(k_0)t} e^{-ik'v_g t} e^{-i\frac{1}{2}\beta k'^2 t} dk'$$

$$= e^{ik_0 x} e^{-\omega(k_0)t} \int_{-\infty}^{+\infty} e^{-ak'^2} e^{ik'x} e^{-ik'v_g t} e^{-\frac{1}{2}i\beta k'^2 t} dk'$$

$$= e^{i[k_0 x - \omega(k_0)t]} \int_{-\infty}^{+\infty} e^{-ak'^2} e^{i[k'(x - v_g t)]} e^{-ik'^2\beta \frac{t}{2}} dk'$$

$$= e^{i[k_0 x - \omega(k_0)t]} \int_{-\infty}^{+\infty} e^{-\left(a + \frac{i\beta t}{2}\right)k'^2} e^{ik'(x - v_g t)} dk'$$

This equations looks like eqn. ② with a replaced by $[a + i\beta t/2]$ and x replaced by $x - v_g t$.

$$\therefore \psi(x,t) = e^{i[k_0 x - \omega(k_0)t]} \sqrt{\frac{\pi}{a + i\beta t/2}}\; e^{-\frac{(x-v_g t)^2}{4(a+i\beta t/2)}}.$$

$$\therefore |\psi(x,t)|^2 = \sqrt{\frac{\pi^2}{(a^2 + \beta^2 t^2/4)}}\; e^{-\frac{(x-v_g t)^2}{2\left(a + \frac{\beta^2 t^2}{4a}\right)}} \quad \text{...... ④}.$$

Equation ④ represents a propagating wave packet with its peak moving with velocity v_g. Comparing eqn ④ with eqn ②A we notice that the quantity a at $t=0$ is replaced by $\left[a^2 + \frac{\beta^2 t^2}{4}\right]^{1/2}$ at time t. So the width of the wavepacket grows larger as it propagates i.e, the wavepacket spreads as it propagates.

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Problem:- IMP Find $\psi(x,0)$ for a Gaussian wave packet $\phi(k) = A\exp\left[-a^2\frac{(k-k_0)^2}{4}\right]$ where A is normalization constant. Calculate the Probability of finding the particle in the region $-a/2 \le x \le a/2$.

Solution:-

$$\int_{-\infty}^{+\infty} |\phi(k)|^2 dk = 1$$

$$\Rightarrow |A|^2 \int_{-\infty}^{+\infty} \exp\left[-\frac{a^2}{2}(k-k_0)^2\right] dk = 1$$

Let $z = k - k_0$.

Gamma Integral

$$\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{\alpha^{n+1}}$$

$$\Rightarrow dz = dk$$

$$\Rightarrow |A|^2 2\int_{0}^{+\infty} \exp\left[-\frac{a^2 z^2}{2}\right] dz = 1$$

Let $\frac{a^2 z^2}{2} = p \quad \therefore \frac{a^2}{2} 2z\, dz = dp$

$$\Rightarrow dz = \frac{dp}{a^2 z} = \frac{dp\, a}{a^2\sqrt{2p}} = \frac{dp\, p^{-1/2}}{\sqrt{2}\, a}.$$

$$\therefore |A|^2 \int_{-\infty}^{+\infty} e^{-p} \frac{1}{\sqrt{2}a} \cdot p^{-1/2} dp = 1$$

$$\Rightarrow \frac{|A|^2 2}{\sqrt{2}a} \int_{0}^{+\infty} e^{-p} p^{-1/2} dp = 1$$

$$\Rightarrow \frac{\sqrt{2}|A|^2}{a} \Gamma\left(\frac{1}{2}\right) = 1$$

$$\Rightarrow \frac{\sqrt{2}\sqrt{\pi}}{a}|A|^2 = 1$$

$$\Rightarrow |A|^2 = \frac{a}{\sqrt{2\pi}}.$$

$$\therefore |A| = \frac{\sqrt{a}}{\sqrt{\sqrt{2\pi}}} = \left(\frac{a^2}{2\pi}\right)^{1/4}$$

$$\therefore \phi(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} \exp\left[-\frac{a^2}{4}(k-k_0)^2\right].$$

$$\therefore \psi_0(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{a^2}{2\pi}\right)^{1/4} e^{-\frac{a^2}{4}(k-k_0)^2 + ikx}\, dk.$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{a^2}{2\pi}\right)^{1/4} e^{-\frac{a^2}{4}(k-k_0)^2}\, e^{i(k-k_0)x}\, e^{ik_0x}\, dk.$$

Now

$$\cancel{-\frac{a^2}{4}(k-k_0)^2 + ikx = -\left[\frac{a^2}{4}(k-k_0)^2 - ikx\right]}$$

Let $k' = k - k_0 \therefore dk' = dk.$

$$\therefore \psi_0(x) = \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4} \int_{-\infty}^{+\infty} e^{-\frac{a^2k'^2}{4}}\, e^{ik'x}\, e^{ik_0x}\, dk'$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4} e^{ik_0x} \int_{-\infty}^{+\infty} e^{-\frac{a^2k'^2}{4} + ik'x}\, dk'$$

Now

$$-\frac{a^2k'^2}{4} + ik'x = -\left[\frac{a^2k'^2}{4} - ik'x\right]$$

$$= -\left[\left(\frac{ak'}{2}\right)^2 - 2\,\frac{ak'}{2}\cdot\frac{ix}{a} + \left(\frac{ix}{a}\right)^2 + \frac{x^2}{a^2}\right]$$

$$= -\left[\left(\frac{ak'}{2} - \frac{ix}{a}\right)^2 + \frac{x^2}{a^2}\right]$$

$$= -\left(\frac{ak'}{2} - \frac{ix}{a}\right)^2 - \frac{x^2}{a^2}.$$

Let $y = \frac{ak'}{2} - \frac{ix}{a}$

$\Rightarrow dy = \frac{a}{2}dk' \Rightarrow dk' = \frac{2}{a}dy$

$$\therefore \psi_0(x) = \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4} e^{ik_0x}\,\frac{2}{a}\int_{-\infty}^{+\infty} e^{-x^2/a^2}\int_{-\infty}^{\infty} e^{-y^2}dy$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4}\frac{2}{a}\,e^{ik_0x}\,e^{-x^2/a^2}\sqrt{\pi}.$$

$$\left[\text{where} \int_{-\infty}^{+\infty} e^{-y^2}dy = \sqrt{\pi}\right].$$

$$\therefore \psi_0(x) = \frac{\cancel{\sqrt{\pi}}}{\sqrt{2}\,\cancel{\sqrt{\pi}}}\,\frac{\sqrt{a}}{(2\pi)^{1/4}}\cdot\frac{2}{a}\,e^{ik_0x}\,e^{-x^2/a^2}$$

$$= \frac{\sqrt{2}}{\sqrt{a}}\cdot\frac{1}{2^{1/4}\pi^{1/4}}\,e^{ik_0x}\,e^{-x^2/a^2}$$

$$= \frac{2^{1/4}}{\pi^{1/4}a^{1/2}}\,e^{ik_0x}\,e^{-x^2/a^2}$$

$$\boxed{\psi_0(x) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{ik_0x}\,e^{-x^2/a^2}}$$

where e^{ik_0x} is the phase of $\psi_0(x)$.

IMP Thus the fourier transform of a Gaussian wave packet is also a Gaussian wavepacket

Solution to part b :- The probability of finding the particle in the region $-a/2 \le x \le a/2$

$$P = \int_{-a/2}^{+a/2} |\psi_0(x)|^2 dx = \sqrt{\frac{2}{\pi a^2}}\int_{-a/2}^{+a/2} e^{-2x^2/a^2}dx$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-1}^{+1} e^{-z^2/2}dz \simeq \frac{2}{3}$$

Problem:- Find $\phi(k)$ for a square wave packet

$$\psi_0(x) = \begin{cases} A e^{ik_0 x} & |x| \leq a \\ 0 & |x| > a \end{cases}$$

Find the factor A so that $\psi(x)$ is normalised.

Solution:- $\int_{-\infty}^{+\infty} |\psi_0(x)|^2 dx = 1$

$$\Rightarrow |A|^2 \int_{-a}^{+a} e^{-ik_0 x} e^{ik_0 x} dx = 1$$

$$\Rightarrow |A|^2 \int_{-a}^{+a} dx = 1$$

$$\Rightarrow 2a|A|^2 = 1 \quad \Rightarrow \quad A = \frac{1}{\sqrt{2a}}.$$

$$\therefore \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi_0(x) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{ik_0 x} e^{-ikx} dx$$

$$= \frac{1}{2\sqrt{\pi a}} \int_{-a}^{+a} e^{i(k_0 - k)x} dx$$

$$= \frac{1}{\sqrt{\pi a}} \frac{\sin[(k-k_0)a]}{k-k_0}.$$